STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 145969

TO: Ben Sackey **Location: 5c31/5c18** **Art Unit: 1626** **Monday, February 28, 2005** **Case Serial Number: 10/684726**	**From: Noble Jarrell** **Location: Biotech-Chem Library** **Rem 1B71** **Phone: 272-2556** **Noble.jarrell@uspto.gov**

Search Notes

=> b reg
FILE 'REGISTRY' ENTERED AT 12:24:33 ON 28 FEB 2005
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STRUCTURE FILE UPDATES: 27 FEB 2005 HIGHEST RN 838819-79-7
DICTIONARY FILE UPDATES: 27 FEB 2005 HIGHEST RN 838819-79-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

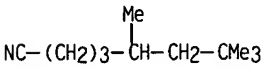
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l13

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN **681449-57-0** REGISTRY
CN **Octanenitrile, 5,7,7-trimethyl- (9CI)** (CA INDEX NAME)
FS 3D CONCORD
MF **C11 H21 N**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP
(Properties); USES (Uses)



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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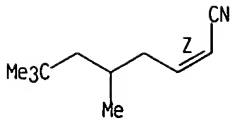
L26 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN **681449-58-1** REGISTRY
CN **2-Octenenitrile, 5,7,7-trimethyl-, (2Z)- (9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF **C11 H19 N**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



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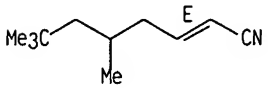
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29898-30-4** REGISTRY
CN **2-Octenenitrile, 5,7,7-trimethyl-, (2E)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **2-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)**
FS STEREOSEARCH
MF **C11 H19 N**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



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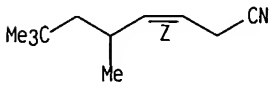
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29680-30-6** REGISTRY
CN **3-Octenenitrile, 5,7,7-trimethyl-, (3Z)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **3-Octenenitrile, 5,7,7-trimethyl-, (Z)- (8CI)**
FS STEREOSEARCH
MF **C11 H19 N**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



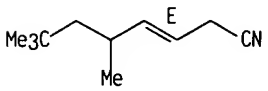
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29680-29-3** REGISTRY

CN **3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **3-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)**
FS STEREOSEARCH
MF **C11 H19 N**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L20 ANSWER 38 OF 38 REGISTRY COPYRIGHT 2005 ACS on STN
RN 372-09-8 REGISTRY
CN **Acetic acid, cyano- (6CI, 8CI, 9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **2-Cyanoacetic acid**
CN **Cyanoacetic acid**
CN **Cyanoethanoic acid**
CN Malonic mononitrile
CN **Monocyanoacetic acid**
CN NSC 5571
FS 3D CONCORD
MF **C3 H3 N O2**
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

NC–CH_2–CO_2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1728 REFERENCES IN FILE CA (1907 TO DATE)
81 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1730 REFERENCES IN FILE CAPLUS (1907 TO DATE)
38 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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(FILE 'HOME' ENTERED AT 11:27:15 ON 28 FEB 2005)

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L2 1 DE2002-10247966/AP,PRN
L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 11:28:48 ON 28 FEB 2005

FILE 'HCAPLUS' ENTERED AT 11:28:49 ON 28 FEB 2005
L4 TRA L3 1- RN : 9 TERMS

FILE 'REGISTRY' ENTERED AT 11:28:49 ON 28 FEB 2005
L5 9 SEA L4

FILE 'WPIX' ENTERED AT 11:28:52 ON 28 FEB 2005
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E DE2002-10247966/AP,PRN
L7 1 DE2002-10247966/AP,PRN
L8 1 L6-7

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L12 5 L11 AND OCTANENITRILE
SEL 2
DEL SEL
SEL RN L12 2
L13 1 E1 AND L12
L14 1844 C9H18O
L15 1582 L14 NOT L10
L16 18 L15 AND OCTANAL
L17 199 C3H3NO2
L18 126 L17 NOT L10
L19 45 L18 AND ACETIC (1A)ACID
L20 38 L19 AND CYANO
L21 1231 C11H19N
L22 1146 L21 NOT L10
L23 112 L22 AND NITRILE
L24 15 L23 AND OCTENENITRILE
L25 13 L24 AND (2 OR 3) (1A) OCTENENITRILE
SEL RN 1 10-12 L25
L26 4 E2-5 AND L25

FILE 'HCAPLUS' ENTERED AT 12:27:07 ON 28 FEB 2005
L27 1 L13
L28 4 L26 OR OCTENENITRILE (3A) TRIMETHYL
L29 3655 L20 OR ACETIC (1A) ACID (1A) CYANO OR (?CYANOACETIC/BI OR CYANO

L30 1 L29 AND L28
L31 1 L27 AND L28
L32 1 L27 OR L30 OR L31

=> b hcap
FILE 'HCAPLUS' ENTERED AT 12:33:00 ON 28 FEB 2005

FILE COVERS 1907 - 28 Feb 2005 VOL 142 ISS 10
FILE LAST UPDATED: 27 Feb 2005 (20050227/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d all fhitstr l32 tot

L32 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:348009 HCAPLUS
DN 140:356957
ED Entered STN: 29 Apr 2004
TI Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel
condensation of **cyanoacetic acid** and isononylaldehyde
followed by catalytic hydrogenation
IN Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal
PA Symrise GmbH & Co. KG, Germany
SO Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DT Patent
LA German
IC ICM C07C255-03
ICS A61K007-46
CC 23-19 (Aliphatic Compounds)
Section cross-reference(s): 46, 62
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413570	A1	20040428	EP 2003-22338	20031004
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10247966	A1	20040506	DE 2002-10247966	20021015
	US 2004127394	A1	20040701	US 2003-684726	20031014
	BR 2003004488	A	20040831	BR 2003-4488	20031014
	JP 2004137275	A2	20040513	JP 2003-354687	20031015
PRAI	DE 2002-10247966	A	20021015		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1413570	ICM	C07C255-03
	ICS	A61K007-46
EP 1413570	ECLA	C07C255/03

DE 10247966 ECLA C07C255/03
US 2004127394 ECLA C07C255/03
JP 2004137275 FTERM 4H003/AB27; 4H003/AC15; 4H003/BA12; 4H003/EA21; 4H003/EB12; 4H003/ED02; 4H003/EE08; 4H003/FA26; 4H006/AA01; 4H006/AA03; 4H006/AB14; 4H059/BA44; 4H059/DA09; 4H059/EA35

AB Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-**Trimethyl**-2(3)-**octenenitriles** which are then subjected to catalytic (e.g., Pd/C) hydrogenation.

ST trimethyloctanenitrile fragrance prepn

IT Nitriles, preparation
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aliphatic, 5,7,7-trimethyloctanenitrile; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT Knoevenagel reaction
(of **cyanoacetic acid** and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octennitriles)

IT Hydrogenation
(of the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octennitriles into 5,7,7-trimethyloctanenitrile)

IT Odor and Odorous substances
(preparation of 5,7,7-trimethyloctanenitrile as)

IT Bleaching agents
Perfumes
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in)

IT Hypochlorites
RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT Nitriles, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(unsatd., Z/E-5,7,7-Trimethyl-2(3)-octennitriles; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation of)

IT **29680-29-3P 29680-30-6P 29898-30-4P 681449-58-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT 7782-50-5, Chlorine, reactions
RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT **681449-57-0P**
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT **372-09-8, Cyanoacetic acid** 1333-74-0, Hydrogen, reactions 49824-43-3, Isononylaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anic Spa; GB 1523028 A 1978 HCAPLUS

(2) Bush Boake Allen Ltd; EP 0017396 A 1980 HCAPLUS

(3) Int Flavors & Fragrances Inc; EP 0347596 A 1989 HCAPLUS

(4) Unilever Plc; EP 0074253 B 1983 HCAPLUS

IT **29680-29-3P**

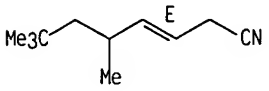
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

RN 29680-29-3 HCAPLUS

CN 3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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L2             1 DE2002-10247966/AP,PRN
L3             1 L1-2

     FILE 'REGISTRY' ENTERED AT 11:28:48 ON 28 FEB 2005

     FILE 'HCAPLUS' ENTERED AT 11:28:49 ON 28 FEB 2005
L4               TRA L3 1- RN :        9 TERMS

     FILE 'REGISTRY' ENTERED AT 11:28:49 ON 28 FEB 2005
L5             9 SEA L4

     FILE 'WPIX' ENTERED AT 11:28:52 ON 28 FEB 2005
L6             1 US20040127394/PN
               E DE2002-10247966/AP,PRN
L7             1 DE2002-10247966/AP,PRN
L8             1 L6-7

=> b hcap
FILE 'HCAPLUS' ENTERED AT 11:29:32 ON 28 FEB 2005
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FILE COVERS 1907 - 28 Feb 2005  VOL 142 ISS 10
FILE LAST UPDATED: 27 Feb 2005  (20050227/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L3   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:348009  HCAPLUS
DN   140:356957
ED   Entered STN:  29 Apr 2004
TI   Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel
     condensation of cyanoacetic acid and isononylaldehyde followed by
     catalytic hydrogenation
IN   Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal
PA   Symrise GmbH & Co. KG, Germany
SO   Eur. Pat. Appl., 7 pp.
     CODEN: EPXXDW
DT   Patent
LA   German
IC   ICM  C07C255-03
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ICS A61K007-46
CC 23-19 (Aliphatic Compounds)
Section cross-reference(s): 46, 62
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI EP 1413570	A1	20040428	EP 2003-22338	20031004	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
DE 10247966	A1	20040506	DE 2002-10247966	20021015	<--
US 2004127394	A1	20040701	US 2003-684726	20031014	<--
BR 2003004488	A	20040831	BR 2003-4488	20031014	<--
JP 2004137275	A2	20040513	JP 2003-354687	20031015	<--
PRAI DE 2002-10247966	A	20021015	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
EP 1413570	ICM	C07C255-03	
	ICS	A61K007-46	
EP 1413570	ECLA	C07C255/03	<--
DE 10247966	ECLA	C07C255/03	<--
US 2004127394	ECLA	C07C255/03	<--
JP 2004137275	FTERM	4H003/AB27; 4H003/AC15; 4H003/BA12; 4H003/EA21; 4H003/EB12; 4H003/ED02; 4H003/EE08; 4H003/FA26; 4H006/AA01; 4H006/AA03; 4H006/AB14; 4H059/BA44; 4H059/DA09; 4H059/EA35	<--

AB Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenenitriles which are then subjected to catalytic (e.g., Pd/C) hydrogenation.

ST trimethyloctanenitrile fragrance prepn

IT Nitriles, preparation
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aliphatic, 5,7,7-trimethyloctanenitrile; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

IT Knoevenagel reaction
(of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octennitriles)

IT Hydrogenation
(of the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octennitriles into 5,7,7-trimethyloctanenitrile)

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(preparation of 5,7,7-trimethyloctanenitrile as)

IT Bleaching agents
Perfumes
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in)

IT Hypochlorites
RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT Nitriles, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(unsatd., Z/E-5,7,7-Trimethyl-2(3)-octennitriles; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation of)

IT 29680-29-3P 29680-30-6P 29898-30-4P 681449-58-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(intermediate; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)
IT 7782-50-5, Chlorine, reactions
RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)
IT 681449-57-0P
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)
IT 372-09-8, Cyanoacetic acid 1333-74-0, Hydrogen, reactions 49824-43-3, Isononylaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
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RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anic Spa; GB 1523028 A 1978 HCAPLUS
(2) Bush Boake Allen Ltd; EP 0017396 A 1980 HCAPLUS
(3) Int Flavors & Fragrances Inc; EP 0347596 A 1989 HCAPLUS
(4) Unilever Plc; EP 0074253 B 1983 HCAPLUS

=> b reg

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 FEB 2005 HIGHEST RN 838086-80-9
DICTIONARY FILE UPDATES: 25 FEB 2005 HIGHEST RN 838086-80-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

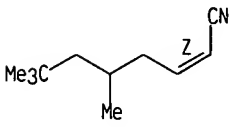
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l5 tot

L5 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **681449-58-1** REGISTRY
CN 2-Octenenitrile, 5,7,7-trimethyl-, (2Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H19 N
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

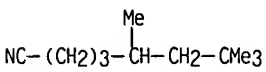
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

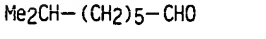
L5 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **681449-57-0** REGISTRY
CN Octanenitrile, 5,7,7-trimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H21 N
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **49824-43-3** REGISTRY
CN Octanal, 7-methyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 7-Methyloctanal
CN Isononylaldehyde
FS 3D CONCORD
MF C9 H18 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMLIST, CSCHEM, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent)

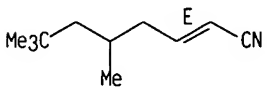


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

29 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
29 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29898-30-4** REGISTRY
CN 2-Octenenitrile, 5,7,7-trimethyl-, (2E)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
FS STEREOSEARCH
MF C11 H19 N
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.

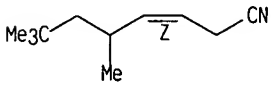


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29680-30-6** REGISTRY
CN 3-Octenenitrile, 5,7,7-trimethyl-, (3Z)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Octenenitrile, 5,7,7-trimethyl-, (Z)- (8CI)
FS STEREOSEARCH
MF C11 H19 N
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



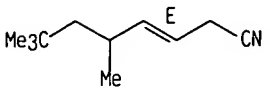
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **29680-29-3** REGISTRY
CN 3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
FS STEREOSEARCH
MF C11 H19 N
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **7782-50-5** REGISTRY
CN Chlorine (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Chlorine mol.
CN Chlorine molecule (Cl2)
CN Diatomic chlorine
CN Dichlorine
CN Molecular chlorine
FS 3D CONCORD
MF Cl2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Cl—Cl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

68006 REFERENCES IN FILE CA (1907 TO DATE)

2274 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
68058 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **1333-74-0** REGISTRY
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dihydrogen
CN Hydrogen (H2)
CN Hydrogen molecule
CN Mol. hydrogen
CN Molecular hydrogen
CN Orthohydrogen
CN Parahydrogen
CN Protium
DR 725200-57-7
MF H2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
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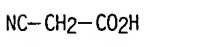
H—H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

295509 REFERENCES IN FILE CA (1907 TO DATE)
3621 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
295705 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **372-09-8** REGISTRY

CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Cyanoacetic acid
CN Cyanoacetic acid
CN Cyanoethanoic acid
CN Malonic mononitrile
CN Monocyanoacetic acid
CN NSC 5571
FS 3D CONCORD
MF C3 H3 N O2
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1728 REFERENCES IN FILE CA (1907 TO DATE)
81 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1730 REFERENCES IN FILE CAPLUS (1907 TO DATE)
38 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> b wpix
FILE 'WPIX' ENTERED AT 11:29:44 ON 28 FEB 2005
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FILE LAST UPDATED: 24 FEB 2005 <20050224/UP>
MOST RECENT DERWENT UPDATE: 200513 <200513/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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HIT STRUCTURES WITHIN THE BIBLIOGRAPHIC DOCUMENT <<<

>>> SMILES and ISOSMILES strings are no longer available as
Derwent Chemistry Resource display fields <<<

>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.
PLEASE CHECK:
http://thomsonderwent.com/support/dwpiref/reftools/classification/code-revision/
FOR DETAILS. <<<

=> d all l8

L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-358450 [34] WPIX
DNC C2004-135920
TI New compound 5,7,7-trimethyloctanonitrile useful for imparting an iris aroma to fragrance compositions and perfumed products, especially bleaches.
DC D21 E16
IN FAHLBUSCH, K; PANTEN, J; SILLON, P; WERNER, M
PA (SYMR-N) SYMRISE GMBH & CO KG; (DRAG-N) DRAGOCO GERBERDING CO GMBH; (FAHL-I) FAHLBUSCH K; (PANT-I) PANTEN J; (SILL-I) SILLON P; (WERN-I) WERNER M
CYC 35
PI EP 1413570 A1 20040428 (200434)* GE 7 C07C255-03
R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV MC MK NL PT RO SE SI SK TR
DE 10247966 A1 20040506 (200434) C07C255-03
JP 2004137275 A 20040513 (200434) 8 C07C255-03
US 2004127394 A1 20040701 (200444) A61K007-46 <--
BR 2003004488 A 20040831 (200460) A61K007-46
CN 1502603 A 20040609 (200460) C07C255-03
ADT EP 1413570 A1 EP 2003-22338 20031004; DE 10247966 A1 **DE 2002-10247966 20021015**; JP 2004137275 A JP 2003-354687 20031015; US 2004127394 A1 US 2003-684726 20031014; BR 2003004488 A BR 2003-4488 20031014; CN 1502603 A CN 2003-1120359 20031015
PRAI **DE 2002-10247966 20021015**
IC ICM A61K007-46; C07C255-03
ICS C07C255-02; C11B009-00; C11D003-395; C11D003-50; D06L003-00
AB EP 1413570 A UPAB: 20041125
NOVELTY - 5,7,7-Trimethyloctanonitrile (I) is new.
DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for:
(1) fragrance composition or perfumed article containing (I);
(2) bleach composition comprising a bleaching agent, (I) and optionally conventional additives.
USE - (I) is useful for imparting an iris aroma to fragrance compositions and perfumed products, especially bleaches based on chlorine and/or hypochlorite.
ADVANTAGE - (I) has iris, vetiver, iris butter, woody and spicy aroma notes and has good stability in aggressive media, especially bleaches.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: D08-B12; D10-A05; E10-A15E

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